Rapid Determination of Benzalkonium chloride in aqueous samples by FTIR spectroscopy in tandem with chemometrics

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Highlights

- The FTIR spectroscopy accompanied by chemometrics methods was carried out for the determination of Benzalkonium chloride in in aqueous samples.
- A genetic algorithm was used as a robust method for wavelength selection.
- The SVM-R and PLS-R regression were used as the calibration model.
- The GA-SVR model represented better static results compared to GA-PLS.

Abstract

In this research, a powerful regression model coupled with FTIR spectroscopy (Mid, 800-1700 cm^{-1}) has been proposed as an efficient method for precise determination of Benzalkonium chloride (BAK) in aqueous samples. For this purpose, both partial least squares regression (PLS-R) and support vector regression (SVR) as methods of multivariate calibration were used for evaluation, and their results were compared. Accordingly, root mean square error of prediction, and leave-one-out cross-validation root mean square error, and correlation coefficients between the calculated (R^2_{cal}) and the predicted (R^2_{pred}) values were used. In comparison to PLS (R^2_{pred} =0.975; RMSEP= 0.321), SVR had a higher R^2_{pred} (0.991) and a lower value of root mean square error of prediction (RMSEP =0.218). The lower detection limit was 0.00068 % w/w for PLS and 0.0011 % w/w for SVR model in a concentration range from 0.013 to 1% w/w. Hence, FTIR spectroscopy combined with SVR can be considered an efficient approach for real-time determination of BAK in aqueous samples.

Keywords: FTIR spectroscopy, Multivariate calibration, Support vector regression, Partial least square regression, Benzalkonium chloride.